Energy Stable SBP-FDTD Methods for Maxwell-Duffing Models in Nonlinear Photonics

Daniel Appelö, Vrushali A. Bokil, Yingda Cheng, and Fengyan Li

Abstract—We consider electromagnetic models that describe nonlinear optical phenomenon in which the nonlinear polarization is driven by the electric field and modeled as an anharmonic oscillator(s). These models are given by Duffing equations and incorporate both nonlinearity and dispersion. Using the auxiliary differential equation approach, our discretization of the coupled Maxwell-Duffing models are high order and energy stable finite difference time domain (FDTD) methods of so called summation by parts (SBP) type. Boundary and interface conditions are handled by the simultaneous approximation technique (SAT).

Index Terms—Summation by parts, simultaneous approximation term, Maxwell-Duffing, Kerr effect, Nonlinear Photonics.

I. INTRODUCTION

Accurate, stable and efficient simulation of wave propagation in optical media is becoming increasingly important as high power lasers become more common both in the laboratory and industrial setting. It is well known that high order accurate methods are more computationally efficient than low (second order and below) order accurate methods to achieve high resolution in many applications. Despite this fact, it is still very common to use the Yee finite difference time domain (FDTD) scheme for electromagnetic computations. A reason for the persisting popularity of the Yee-FDTD scheme is its simplicity combined with its ability to preserve energy on the discrete grid.

In this article, we consider energy stable, staggered and non-staggered finite difference discretizations of Maxwell’s equations in a non-magnetic dispersive nonlinear optical medium using summation by parts operators (SBP) [1]. Using the auxiliary differential equation (ADE) technique [2], we append to Maxwell’s equations constitutive laws involving ordinary differential equations (ODEs) that model the time evolution of the macroscopic polarization (average dipole moment per unit volume). In particular, the nonlinearity appears in the constitutive laws due to the response of the medium to the incident electromagnetic fields, and is only present in the ODEs for the time evolution of the polarization. The polarization models that we consider below, called Duffing models, only contain nonlinearity in the zeroth order term, and we can directly apply to these models the SBP methods developed by Nordström and Gustafsson for Maxwell’s equations in linear and non-dispersive materials [3]. We show that our adaptations to the Maxwell-Duffing nonlinear model are also high order, energy stable and conserve a discrete version of the continuous energy of the nonlinear physical system.

We derive the energy analysis of the SBP method for the semi-discrete system only. In order to preserve a fully discrete energy and in order to achieve a uniformly high order method, time integrators need to be chosen carefully. We note that the second order accurate fully discrete energy stable time discretizations, that we derived in [4], could also be applied to the Maxwell-Duffing models in conjunction with the spatial discretization considered here. In this paper however, we consider both explicit Runge-Kutta and Taylor methods, as well as implicit Runge-Kutta methods based on Gauss-Legendre quadrature. The use of Gauss-Legendre quadrature makes the resulting (collocation) Runge-Kutta method symplectic. Of course, there is no guarantee that a symplectic method will preserve energy exactly (although a nearby energy will be preserved), so we settle for solving the nonlinear system of equations approximately using the so called spectral deferred correction (SDC) method [5], [6]. In SDC the nonlinear system is turned into a fixed point iteration. If the fixed point is found to machine precision, then the SDC solution is the same as the (symplectic) Runge-Kutta solution, but if the iteration is terminated based on order of accuracy consideration, the symplectic property is only approximately satisfied. Despite this approximation and the fact that symplecticity does not imply energy conservation, we demonstrate through numerical examples that (at least for the models considered here) very good energy conservation properties are attainable when SDC methods are used.

To model nonlinearity and dispersion in optical phenomenon, we consider a general class of polarization models called Duffing equations [7]. Historically, the Duffing equation, which is named after Georg Duffing, is a nonlinear second order ODE modeling the free and forced harmonic vibration of an oscillator in which the stiffness force has quadratic and cubic terms [8]. Subsequently, the label Duffing equation has been used to describe any oscillator that has a cubic stiffness term, regardless of the type of damping or excitation [8]. In nonlinear optics, Duffing equations are used to model the polarization accounting for dispersion and nonlinearity related to third order effects in optical and photonic materials. These equations include the finite and retarded response time of the medium and are advantageous in studying the propagation...
characteristics of ultrashort laser pulses [9]. In this paper, we consider a variety of Maxwell-Duffing models and their discretizations by the SBP methods to simulate nonlinear optical phenomenon. In particular, we present the construction of high order in space SBP methods and simultaneous approximation terms, along with high order time discretizations, and we demonstrate the effectiveness of our new discretizations on a variety of test problems.

The rest of the paper is organized as follows. In Section II we introduce the models for simulating nonlinear optical phenomenon, and in Section III, we describe the numerical discretizations. In Section IV, numerical experiments are reported, which are followed by the summary and future work in Section V.

II. MODELS AND CONSTITUTIVE LAWS FOR NONLINEAR OPTICAL MATERIALS

To observe nonlinear effects in common materials, high-intensity light sources, such as lasers, are required, and the particular nonlinear effects observed depend on which term is dominant in the electric polarization [10]. We will consider materials in which the dominant nonlinearities are of the third order (such as optical glass fibers) and include instantaneous as well as delayed material responses.

Using the ADE approach, we append to Maxwell’s partial differential equations (PDEs) a system of ODEs describing the nonlinear relationship between the macroscopic polarization vector field \( \mathbf{P} \) and the electric field \( \mathbf{E} \). Our approach follows the development in [11]. The hybrid system of Maxwell PDEs and auxiliary ODEs are then simultaneously evolved in time.

Maxwell’s equations in a non-magnetic, non-conductive medium \( \Omega \subset \mathbb{R}^d, d = 1, 2, 3, T > 0 \), containing no free charges, govern the dynamic evolution of the electric field \( \mathbf{E} \) and the magnetic field \( \mathbf{H} \). The evolution equations are

\[
\begin{align*}
\mu_0 \partial_t \mathbf{H} + \nabla \times \mathbf{E} &= 0, \quad \text{in } (0, T] \times \Omega, \\
\epsilon_0 \epsilon_{\infty} \partial_t \mathbf{E} + \epsilon_0 \mathbf{J} - \nabla \times \mathbf{H} &= 0, \quad \text{in } (0, T] \times \Omega, \\
\nabla \cdot \mathbf{B} &= 0, \quad \nabla \cdot \mathbf{D} = 0, \quad \text{in } (0, T] \times \Omega,
\end{align*}
\]

(1a) (1b) (1c)

The electric flux density \( \mathbf{D} \), and the magnetic induction \( \mathbf{B} \), are related to the electric field and magnetic field, respectively, via the constitutive laws

\[
\begin{align*}
\mathbf{D} &= \epsilon_0 (\epsilon_{\infty} \mathbf{E} + \mathbf{P}), \\
\mathbf{B} &= \mu_0 \mathbf{H},
\end{align*}
\]

(2)

with the polarization current density, \( \mathbf{J} \), defined as the time derivative of the macroscopic polarization, i.e. \( \mathbf{J} = \partial_t \mathbf{P} \). The parameter \( \epsilon_0 \) is the electric permittivity of free space, while \( \mu_0 \) is the magnetic permeability of free space. The term \( \epsilon_{\infty} \mathbf{E} \) captures the linear instantaneous response of the material to the EM fields, with \( \epsilon_{\infty} \) defined as the relative electric permittivity in the limit of infinite frequencies. The macroscopic (electric) polarization \( \mathbf{P} \) includes both linear and nonlinear effects, and is related to the electric field through different mechanisms depending on the optical phenomenon under consideration. In this work we focus on general Maxwell-Duffing dispersive models.

The Duffing equation, for the electric polarization, models high order effects by including both nonlinearity and dispersion, and can be written in a general form as

\[
\frac{\partial^2 \mathbf{P}}{\partial t^2} + \frac{1}{\tau} \frac{\partial \mathbf{P}}{\partial t} + \omega_0^2 \mathbf{P} \mathcal{F}(\mathbf{P}) = \omega_p^2 \mathbf{E},
\]

(3)

with a range of choices for \( \mathcal{F}(\mathbf{P}) \). Here \( \omega_0 \) and \( \omega_p \) are the resonance and plasma frequencies of the medium, respectively, and \( \tau^{-1} \) is a damping constant. In this paper, we will consider an \( N \)th order polynomial model for the Duffing equation, given as

\[
\mathcal{F}(\mathbf{P}) = \mathcal{F}_{\text{PMD}}(\mathbf{P}) := \sum_{l=0}^{N_{\text{PMD}}} \lambda_{2l} |\mathbf{P}|^{2l},
\]

(4)

with \( N_{\text{PMD}} \in \mathbb{N}, N_{\text{PMD}} \geq 1 \). We refer to the system of equations (1)-(4) as the \( N \)th Order Polynomial Maxwell-Duffing (PMD) model. This includes as special cases the Cubic-Exponential Maxwell-Duffing (C-EMD) model \((N_{\text{PMD}} = 1, \lambda_0 = 1, \lambda_2 = \alpha)\), the Quintic-Exponential Maxwell-Duffing (Q-EMD) model \((N_{\text{PMD}} = 2, \lambda_0 = 1, \lambda_2 = \alpha, \lambda_4 = \alpha^2/2)\), and in general an \( N \)th Order Polynomial Exponential Maxwell-Duffing (P-EMD) model which are all approximations of the Exponential Maxwell-Duffing (EMD) model with \( \mathcal{F}(\mathbf{P}) := \exp(\alpha |\mathbf{P}|^2) \).

We note that the PMD model is more general in that it incorporates the C-EMD, Q-EMD and higher order approximations P-EMD of the EMD, but can also be used with other parameters, \( \lambda_{2l} \), that are not approximations of the EMD, as is suggested by our energy estimates below.

We note that if \( \mathcal{F}(\mathbf{P}) = 1 \), the Duffing model reduces to the linear Lorentz dispersive model. On the other hand, as pointed out in [12], for a specific function form (different than (4)) of \( \mathcal{F}(\mathbf{P}) \), under certain assumptions, the Duffing model (3) will reproduce the Kerr model, another widely used nonlinear model to describe cubic nonlinear effects such as the Kerr effect [13]. We refer the reader to our recent work [14], on the construction of energy stable FDTD approximations of Maxwell’s equations along with the nonlinear Kerr-Raman model for polarization.

The Maxwell-Duffing models need to be closed by initial and boundary conditions on \([0, T] \times \Omega\). Here we will exclusively consider perfect electric conductors (PEC) resulting in homogeneous Dirichlet boundary conditions on the tangential components of the electric field on \( \partial \Omega \), the boundary of the domain \( \Omega \).

A. An Energy Estimate in Two Dimensions

In two dimensions, assuming a transverse electric mode, the electric field, \( \mathbf{E} = (E^x, E^y) \), and polarization, \( \mathbf{P} = (P^x, P^y) \), have two components each that are incident in the \((x, y)\) plane, while the magnetic field has one component, \( H^z \), transverse to the electric field out of this plane. Using the polarization current density \( \mathbf{J} = (J^x, J^y) \), and assuming the Duffing model (3) to be damping-free \((\tau^{-1} = 0)\), we rewrite equation (3) in first order form as

\[
\frac{\partial \mathbf{J}}{\partial t} = -\omega_0^2 \mathbf{P} \mathcal{F}_{\text{PMD}}(\mathbf{P}) + \omega_p^2 \mathbf{E}.
\]

(5)

We assume the PEC boundary conditions for the electric field on \( \partial \Omega \). An energy identity for this model can be obtained.
using the energy method as follows. Multiplying (5) by \( \varepsilon_0 / \omega_p^2 \), multiplying each equation in (1a), (1b) and (5) by appropriate quantities and summing over the domain, taking norms, together with integration by parts in (1b), we obtain the energy identity

\[
\frac{d}{dt} \mathcal{E}(t) = 0,
\]

where, the time dependent energy of the PDM model denoted as \( \mathcal{E}(t) \) is defined as

\[
\mathcal{E}(t) := \mu_0 \| H \|^2 + \varepsilon_0 \varepsilon_\infty \| E \|^2 + \frac{\varepsilon_0}{\omega_p^2} \| J \|^2 + \frac{\varepsilon_0}{\omega_p^2} \| \mathbf{P} \|^2 + \frac{\varepsilon_0}{\omega_p^2} \| J \|^2.
\]

Equation (6) implies that the energy \( \mathcal{E} \) is constant in time. Here \( \| \cdot \| \) is the standard \( L_2 \) norm with respect to the spatial domain, induced by the standard \( L_2 \) inner product \((\cdot, \cdot)\). Note that the damped case can be treated analogously but that \( \mathcal{E}'(t) \leq 0 \) in the presence of damping \((\tau^{-1} \neq 0)\).

### III. Numerical Methods

#### A. Summation by parts (SBP) finite difference methods

The main idea behind summation by parts finite differences is to design difference approximations that mimic the integration by parts formula, which in one dimension on \([x_L, x_R] \subset \mathbb{R}\), can be written as

\[
\int_{x_L}^{x_R} u(x)v(x)dx = -\int_{x_L}^{x_R} u(x)v(x)dx + v(x_R)u(x_R) - v(x_L)u(x_L),
\]

so that the energy analysis of the continuous problem can be directly applied to the semi-discretization (in space) of the governing equations at hand.

As an illustrative example of deriving an energy identity, consider the one dimensional linear version of the PMD model with \( N_{PMD} = 0 \), \( \lambda_0 = 1 \), governing the electric and magnetic fields, \( E \) and \( H \), in a non-magnetic dispersive optical medium. From (1)-(3), we have the following one dimensional model,

\[
\varepsilon_0 \varepsilon_\infty E_t = H_x - \varepsilon_0 J, \quad \mu_0 H_t = E_x, \quad P_t = J, \quad J_t = -J/\tau - \omega_p^2 P + \omega_p^2 E.
\]

Following similar steps as in the 2D case above we arrive at an energy identity. In particular, multiplying the above equations by suitable quantities and integrating over the domain \( \Omega \) we obtain the equations

\[
(\varepsilon_0 \varepsilon_\infty E, E_t) = (E, H_x) - \varepsilon_0 (E, J),
\]

\[
(\mu_0 H, H_t) = (H, E_x),
\]

\[
\varepsilon_0 \varepsilon_\infty \omega_p^2 (P, P_t) = \varepsilon_0 \varepsilon_\infty \omega_p^2 (P, J),
\]

\[
\varepsilon_0 \omega_p^2 (J, J_t) = -\varepsilon_0 \omega_p^2 (J, J) - \mu_0 \omega_p (P, J) + \varepsilon_0 (J, E).
\]

Summing up these equations we have

\[
\frac{d}{dt} \left( \varepsilon_0 \varepsilon_\infty \| E \|^2 + \mu_0 \| H \|^2 + \varepsilon_0 \varepsilon_\infty \| E \|^2 \right) + \frac{\varepsilon_0}{\omega_p^2} \| P \|^2 + \frac{\varepsilon_0}{\omega_p^2} \| J \|^2
\]

\[
= (E, H_x) + (E, H) - \varepsilon_0 \omega_p (P, J) + \varepsilon_0 (J, E).
\]

Here the last equality follows from an integration by parts (IBP) in either of the terms \((E, H_x), (E, H)\).

The above energy estimate implies that, given suitable boundary conditions on \( E \) and \( H \) (for example \( E = 0 \) on the boundary), the initial boundary value problem is well-posed, i.e. the solution depends continuously on data, see e.g. [15].

Finite difference operators with the SBP property satisfy a discrete version of the continuous IBP formula (8). Precisely, given vector approximations \( E^h, H^h \in \mathbb{R}^{n+1} \) to \( E \) and \( H \), defined on a grid \( x_i = x_{L} + ih, i = 0, \ldots, n, h = (x_R - x_L)/n \), SBP operators for the first derivatives \( D \equiv R^{-1}Q \) are constructed so that

\[
(E^h)^T R D H^h + (H^h)^T R D E^h = E^h H^h - E_0^h H_0^h.
\]

Here \( R \) is a diagonal and positive definite matrix defining an inner product (and the induced norm), \( Q \) is a matrix with the property \( Q + Q^T = \varepsilon_i e_i e_i^T - \varepsilon_0 e_0 e_0^T \), with \( e_j \) being the \( j \)th unit vector. For the actual construction of SBP operators, we refer readers to the original paper by Kreiss and Scherer [16], and the paper by Strand [17], that contain many of the early operators and the more recent review by Svärd [11]. Here, we simply assume that SBP operators exist. Next, we illustrate how these SBP operators can be used to simulate nonlinear optics problems in an accurate and stable manner.

The energy analysis is not changed by lower order terms. Thus, we illustrate the semi-discrete energy analysis using SBP operators for the linear one dimensional problem (9) by suppressing the lower order terms in (9a). Using an SBP operator \( D \) to approximate \( \partial / \partial x \) we obtain

\[
\varepsilon_0 \varepsilon_\infty E_t^h = D H^h, \quad \mu_0 H_t^h = D E^h,
\]

to approximate (9a)-(9b). Multiplying the above equations by \((E^h)^T R \) and \((H^h)^T R \) respectively, followed by adding the resulting equations we find

\[
\frac{d}{dt} \left( \varepsilon_0 \varepsilon_\infty \| E^h \|^2 + \mu_0 \| H^h \|^2 \right) = E_n^h H_n^h - E_0^h H_0^h.
\]

The above equality illustrates that the change of energy is controlled by the approximations to the electric and magnetic fields on the boundary. Below we discuss how to chose penalty terms to handle interface coupling and physical boundary conditions. A schematic of the computational setup can be found in Figure 1.

#### 1) Interfaces: Consider an interface between two grids with \( E^{+h}, H^{+h}, E^{-h}, H^{-h} \) denoting the approximations to the right and to the left of the interface. To couple the two domains we add “zeros”, so called Simultaneous Approximation Terms (SAT), [18], to the approximation of the governing equations.
is potentially because the SAT terms only apply at the domain \( \gamma \) the difference between the choices of \( \beta > 0 \).

**Remark 3.1:** The structure of the simultaneous approximation term is similar to the numerical flux in discontinuous Galerkin (DG) methods, in which the parameter \( \gamma = 0.5 \) and alternating fluxes \( (\gamma = 0 \text{ or } 1) \) and the parameter \( \beta \) adds an upwind component to the numerical flux. In DG methods the choice of numerical flux can have significant effect on the overall accuracy of the method but here, as illustrated in the numerical experiments, the difference between the choices of \( \gamma \) and \( \beta \) is small. This is potentially because the SAT terms only apply at the domain boundary, unlike in DG schemes, the flux terms appear in all cell boundaries.

**4) Multiple dimensions:** The generalization of the above procedure to multiple dimensions is straightforward on Cartesian meshes as it can be applied line-by-line in each dimension. Extensions to structured curvilinear meshes is also direct (see e.g. [19]) but will not be pursued here. Finally, as the nonlinearities we consider here only contain undifferentiated terms, they are naturally handled by the time integrators discussed below.

**B. Staggered summation by parts finite differences**

Traditionally SBP finite differences have been restricted to non-staggered grids but recently O’Reilly and co-authors [20], [21], [22] have shown that SBP operators can also be formulated on staggered grids. Given the popularity of the staggered Yee scheme we also consider discretizations using staggered SBP operators. However, we note that the extension of staggered SBP operators to curvilinear grids is challenging and we will therefore limit the discussion here to one dimensional problems.

Define the staggered grids \( x_+ = [x_0, x_1, \ldots, x_{n-1}, x_n] \) and \( x_- = [x_0, x_{1/2}, \ldots, x_{n-1/2}, x_n] \). On these grids SBP operators, \( D_+ \equiv R_+^T P + \sigma \) and \( D_- \equiv R_-^T P - \sigma \) can be derived, [20]. Again, \( R_+ \) and \( R_- \) are diagonal matrices and \( D_+ \) and \( D_- \) approximate the derivatives on the grid \( x_+ \) using values from \( x_- \) and vice versa. A crucial property of the operators is that they satisfy the SBP identity:

\[
Q_+ + Q_- = (e_n e^T_n - e_0 e^T_0).
\]

As above, let \( \{E^h, P^h, J^h\} \) and \( H^h \) be grid functions approximating \( \{E, P, J\} \) and \( H \), on the \(-\) and \(+\) grids respectively. We then approximate the derivatives according to

\[
E_x \approx D_- E^h + \sigma R_+ e_n E^h + \sigma_0 R_+ e_0 E^h; \quad H_x \approx D_+ H^h.
\]

Resulting in the semi-discretization:

\[
\begin{align*}
\epsilon_0 e^\infty E^h_t &= (D_+ H^h - \epsilon_0 J^h), \quad (13a) \\
\mu_0 H_t &= (D_- E^h + \sigma R_+ e_n E^h + \sigma_0 R_+ e_0 E^h), \quad (13b) \\
J^h_t &= -J^h / \tau - \omega_0^2 P^h + \omega_0^2 E^h. \quad (13c)
\end{align*}
\]

To derive a semi-discrete estimate we multiply (13a)-(13d) by \( (E^h)^T R_+ \), \((H^h)^T R_+ \), \((P^h)^T R_+ \) and \((J^h)^T R_+ \), respectively, and add them up. The, using (12), the discrete energy identity becomes

\[
\frac{1}{2} \frac{d}{dt} \left( \epsilon_0 e^\infty (E^h)^T R_+ E^h + \mu_0 (H^h)^T R_- H^h \\ + \frac{\epsilon_0 \omega_0^2}{\omega_0^2} (P^h)^T R_+ P^h + \frac{\epsilon_0}{\omega_0^2} (J^h)^T R_+ J^h \right) = \frac{\epsilon_0}{\omega_0^2} (J^h)^T R_+ J^h + (\sigma_n + 1) H^h E^h + (\sigma_0 - 1) H_0^h E^h_0.
\]

An obvious choice for the penalty parameters is \( \sigma_n = -1 \) and \( \sigma_0 = 1 \). This yields an energy conserving discretization when the relaxation time is \( \tau = \infty \).
C. Time discretizations

After semi-discretization in space using SBP operators, the evolution equations take the form of a system of ODEs \( y'(t) = f(y(t), t) \), \( y(0) = y_0 \). This system can be formally solved by integrating in time

\[
y(\Delta t) - y_0 = \int_0^{\Delta t} f(y(\tau), \tau) \, d\tau,
\]

where, \( \Delta t > 0 \) is a suitable time step. The Picard form (14) can be turned into a time discrete numerical method by approximating the integral using numerical quadrature. This procedure results in implicit Runge-Kutta methods that require the resulting nonlinear system of equations to be solved at each time step. Here we employ so called spectral deferred correction (SDC) methods [5], on the form analyzed in [6] to iteratively solve these non-linear equations. This solve is done at each iteration in which the candidate solution is improved by evolving the correction using the forward Euler method with time steps corresponding to the distance between the quadrature points (note that an implicit or implicit-explicit method could also be used for the correction, see [6] for details). When using a \( s \)-point Gauss-Legendre quadrature, it was shown in [6], that the error in the fixed point iteration is accurate to order \( 2s \) after \( 2s - 1 \) corrections. Unless explicitly stated, this is how many iterations we will use in our numerical computations below. We note that, as the non-linear system of equations is only solved approximately, the symplectic properties of the Gauss-Legendre Runge-Kutta method will, in general, be lost. Using additional corrections improves the symplectic properties but does not increase the order of accuracy. An advantage with SDC methods compared to explicit Runge-Kutta methods is that they easily can attain high order of accuracy. In addition, since we exclusively use forward Euler for the correction iteration the complexity and implementation of the method is very similar to an explicit method.

Of course as our discretization is of method-of-lines type other time integrators may also be used. For example, in some of the numerical examples below we use the classic fourth order Runge-Kutta method as well as Taylor series.

The constraints on the allowable timesteps depend both on which SBP operator that is used and on the time stepping method. Typically, increasing the order of accuracy of the SBP operators reduces the timestep slightly while increasing the order of the timestep increases the allowable timestep linearly with order. The constraint on the timesteps for the methods we propose are, in general, slightly stricter than for traditional FDTD.

IV. Numerical Examples

A. Non-staggered discretization in two dimensions

In this section, we present numerical examples using non-staggered SBP operators in two dimensions. To this end, we will use the sixth order accurate in the interior and third order accurate on the boundary operator by Strand [17] and choose the free parameter \( x_3 = 0.70127127127127 \) (defined in [17]). It is known, see e.g. [1], that the order of accuracy of this SBP operator is 4 in the \( L_2 \) norm. Note that we used normalized units until the very last numerical example.

1) Self convergence: To test our method and implementation we perform a self convergence study for a single material using the PMD model with parameters \( \mu_0 = 1.2, \varepsilon_0 = 1.1, \varepsilon_\infty = 1.0, \tau = \infty, \omega_0^2 = 1.5, \omega_\infty^2 = 1.2, N_{PMD} = 2, \lambda_0 = 1, \lambda_2 = 1, \lambda_3 = 100 \). The computational domain is the square \((x, y) \in [-3/2\pi, 3/2\pi]^2\).

At the initial time all the fields are set to zero except \( H_z \) which we take to be the trigonometric function

\[
H_z(x, y) = \sin(x) \sin(y).
\]

We evolve the solution until time \( t = 1 \) and compute the error in \( E_x \) (the other fields have very similar behavior) on a grid with \( h = 3\pi/40 \) against a reference solution with \( h = 3\pi/1280 \). To evolve in time we use a sixth order accurate “explicit” SDC method with Gauss-Legendre nodes with a time step \( \Delta t \approx 0.3h \). The results, which can be found in Table I, clearly shows that the method is fourth order accurate.

2) Energy Conservation: We repeat the same computation as in the previous convergence study but set the final simulation time to be \( t = 50 \) and compare the preservation of the discrete SBP version of the energy \( E(t) \) from (7). In Figures 2, the difference in energy between two subsequent time steps is plotted using SDC with 1, 2 and 3 Gauss-Legendre nodes. As discussed above the underlying Gauss Runge-Kutta methods are symplectic, their SDC approximation is not, and neither is guaranteed to preserve a general energy. This can be observed in Figure 2 which illustrates that the conservation of energy increases with increasing order of accuracy.

3) Behavior at longer times and stronger nonlinearity: Next we perform simulations until time \( t = 200 \), on the same domain as above and with the same initial data but with the material parameters \( \mu_0 = 1.2, \varepsilon_0 = 1, \varepsilon_\infty = 1, \tau = \infty, \omega_0^2 = 16, \omega_\infty^2 = 16, \lambda_0 = 1, \lambda_2 = 0 \). This corresponds to the
linear Lorentz model. We control the nonlinearity by changing $\lambda_4$, i.e. by changing to the PMD model with $N_{PMD} = 2$. Here we are interested in demonstrating the generation of higher harmonics as the nonlinearity controlled by $\lambda_4$ is increased according to $\lambda_4 = 0, 1, 10, 100$. To keep the error in the solution small we use grids with $161^2$ grid-points for the first three values of $\lambda_4$, and $321^2$ for the last value. We note here that the larger number of gridpoints required for the larger nonlinearity is not due to stability but due to the smaller length and timescales created by the stronger nonlinearity. We also use 3 Gauss-Legendre nodes in the SDC for the three first values and 5 nodes for the last. In Figure 3 we display the $E_x$ field sampled in a point 1/4 along the diagonal from the lower left to the upper right corner. The displayed solution is for the last 15 time units in the computation and for the different values of $\lambda_4$. The figure shows how the larger values of $\lambda_4$, corresponding to stronger nonlinearity, introduces small oscillations. To quantify this further we perform a Fourier transform of the signals and plot the spectrum, see Fig. 3.

For the linear model with $\lambda_4 = 0$ there are two primary frequencies, the Duffing (anharmonic) oscillator and the standing wave solution of the free space Maxwell’s equations. These are clearly displayed in the blue line in Figure 3. For the smallest value, $\lambda_4 = 1$, there are only a few new harmonics generated, two of them being in-between the two primary frequencies but for the larger values of $\lambda_4$ there is a significant and more uniform generation of harmonics. However, even for the largest nonlinearity, the solution at the final time is very close to a standing mode of the free space problem.

**B. Evolution of a pulse in different materials**

To demonstrate some different wave propagation behaviors that can be modeled by the Maxwell-Duffing models we consider the evolution of a simple initial data consisting of a magnetic monopole

$$H_z(x, y, 0) = \exp(-36(x^2 + y^2)).$$

The computations are performed on a square domain $(x, y) \in [-2, 2]^2$ using a fine grid with $h = 4/500$ and a 10th order SDC method. The initial data is sampled until time $t = 2$ when we take a snapshot of the $H_z$ field.

The different materials we consider are $(A)$ Maxwell’s equations in free space with $\mu_0 = 1.2, \varepsilon_0 = 1, \varepsilon_{\infty} = 1$, $(B)$ a linear Lorentz dispersive model with $\omega_0^2 = 1, \omega_p^2 = 1$, and $\lambda_0 = 1$, $(C)$ a linear Lorentz dispersive model with $\omega_0^2 = 1, \omega_p^2 = 1000$, and $\lambda_0 = 1$, and $(D)$ a nonlinear PMD model with $\omega_0^2 = 1, \omega_p^2 = 1, \lambda_0 = 1$ and $\lambda_4 = 1000$.

In the four quadrants of Figure 4 we display the solution at the final time for the four different materials. The solution in $(A)$ displays the usual non-dispersed outgoing cylindrical shape traveling at speed 1. The main difference between the slightly dispersive solution in $(B)$ and the non-dispersive solution in $(A)$ is that there is a slight residue of the initial data in the wake of the wave.

For the material $(C)$ the frequency combination makes the wave essentially non-propagating with the shape of the solution at the final time being very close to the initial data but with an amplitude that has decreased to 0.75 from 1. If this material becomes nonlinear, as in $(D)$, there are again propagating wavefronts that travel at a much smaller speed. In addition the wave fronts are much more concentrated with the larger wave traveling faster than the smaller wave.

In terms of performance we note that for the solution to above problem each degree of freedom took around 0.2$\mu$s to advance one timestep on a MacBook Pro (2017) with an Intel Core i7 3.5 GHz processor. The code is written in modern Fortran and compiled with -03 optimization.

1) **Multi-block method: self convergence:** To study the convergence properties for the coupled solver, we simulate Maxwell’s equations with material constants set to unity in a domain consisting of three blocks coupled by the interface conditions discussed in Section III, of unit size and with the lower left corner of the left-most block in $(-1, 0)$. The blocks thus occupy the domain $(x, y) \in [-1, 2] \times [0, 1]$. The initial data is taken to be zero for all fields but for $H_z$ which we take to be

$$H_z(x, y, 0) = \exp(-144(x^2 + (y - 0.5)^2)).$$

The initial data is evolved for 5 time units and we compute the error at the final time in the $H_z$ field using a reference solution obtained with $h = 1/640$. We report the $L_2$ errors for solutions on grids with $h = 1/20, 1/40, 1/80$ and 1/160.
Throughout the experiments with the multi-block method we use the classic Runge-Kutta method of order four and in this experiment we set the time step to be $\Delta t = 0.6h$.

### Table II

**Self convergence of the multi-block solver for Maxwell’s equations in a non polarized material with $\beta = 0$, $\gamma = 1$ (top), data is for $\beta = 0$, $\gamma = 0.5$ (middle), and $\beta = 0.5$, $\gamma = 0.5$ (bottom).**

<table>
<thead>
<tr>
<th>$h$</th>
<th>1/20</th>
<th>1/40</th>
<th>1/80</th>
<th>1/160</th>
<th>1/320</th>
</tr>
</thead>
<tbody>
<tr>
<td>$L_2$-err.</td>
<td>2.28(-2)</td>
<td>5.75(-3)</td>
<td>3.53(-4)</td>
<td>1.03(-5)</td>
<td>6.03(-7)</td>
</tr>
<tr>
<td>Rate</td>
<td>1.99</td>
<td>4.03</td>
<td>5.10</td>
<td>4.09</td>
<td></td>
</tr>
<tr>
<td>$L_2$-err.</td>
<td>2.35(-2)</td>
<td>4.99(-3)</td>
<td>2.94(-4)</td>
<td>8.87(-6)</td>
<td>6.61(-7)</td>
</tr>
<tr>
<td>Rate</td>
<td>2.25</td>
<td>4.07</td>
<td>5.04</td>
<td>3.75</td>
<td></td>
</tr>
<tr>
<td>$L_2$-err.</td>
<td>2.20(-2)</td>
<td>4.33(-3)</td>
<td>1.81(-4)</td>
<td>7.20(-6)</td>
<td>4.73(-7)</td>
</tr>
<tr>
<td>Rate</td>
<td>2.34</td>
<td>4.60</td>
<td>6.65</td>
<td>3.93</td>
<td></td>
</tr>
</tbody>
</table>

In Table II we report the errors and the observed rates of convergence (computed as the base 2 logarithm of the ratios of the errors in subsequent grid refinements) for different combinations of $\gamma$ and $\beta$ in the SAT. The two uppermost results are for energy conserving ($\beta = 0$) discretizations and would correspond to alternating and central flux in a DG setting. Here, unlike in the DG setting where alternating fluxes typically outperforms central fluxes, the difference between alternating ($\gamma = 1$) and central ($\gamma = 0.5$) averaging is not very pronounced in either the absolute error levels or the rates of convergence. The addition of a slight penalization of a jump at the interface between blocks ($\beta > 0$) also does not appear to impact the overall error levels much.

### Table III

**Self convergence for a nonlinear model. Here $\beta = 0$, $\gamma = 0.5$.**

<table>
<thead>
<tr>
<th>$h$</th>
<th>1/20</th>
<th>1/40</th>
<th>1/80</th>
<th>1/160</th>
<th>1/320</th>
</tr>
</thead>
<tbody>
<tr>
<td>$L_2$-err.</td>
<td>1.58(-2)</td>
<td>4.41(-3)</td>
<td>2.89(-4)</td>
<td>8.45(-6)</td>
<td>5.19(-7)</td>
</tr>
<tr>
<td>Rate</td>
<td>1.84</td>
<td>3.93</td>
<td>5.10</td>
<td>4.03</td>
<td></td>
</tr>
</tbody>
</table>

Finally, in Table III we repeat the above self convergence experiment in a nonlinear material with $\omega_f^2 = 16$, $\omega_p^2 = 16$ and $\lambda_0 = 1$ in all blocks and with $\lambda_2 = \lambda_4 = 1$ and $\lambda_2 = \lambda_4 = 2$ in the middle and rightmost block respectively ($\lambda_2$ and $\lambda_4$ are zero in the leftmost block). The results do not differ much from those obtained in a non-polarized material confirming that the high order of accuracy of the proposed method also holds in the presence of nonlinearity.

2) **Multi-block domain: a nonlinear waveguide.** As an example with multiple blocks we consider a waveguide like structure occupying the domain $(x, y) \in [0, 5] \times [0, 1]$ which we discretize with 5 blocks of unit size with Cartesian equidistant grids with grid size $h = 1/400$. Time-stepping is the same as in the previous example. Throughout we set $\mu_0 = \varepsilon_0 = \varepsilon_\infty$ and in the domain $(x, y) \in [2, 3] \times [0, 1]$ we place a material with $\omega_0^2 = 1$, $\omega_p^2 = 1000$, $\lambda_1 = 1$, and $\lambda_2 = 10$.

To illustrate the effect of the nonlinear material for different frequencies we add the solenoidal forcing

$$
\begin{pmatrix}
  y - 0.5 \\
  0.5 - x
\end{pmatrix}
50^2 \sin(\omega t)e^{-200(|x-0.5|^2+(y-0.5)^2)}
$$

to the evolution equations for equations for $(E_x, E_y)^T$. The simulation is started from rest and we impose PEC boundary conditions on all sides.

In Figure 5 we display the $H_z$ field at time $t = 5$ for $\omega = 20, 35$ and 50. It is clear that the nonlinear material acts as a pass filter that effectively blocks lower frequencies and allows higher frequencies to propagate. In addition the nonlinear inset appears to make the waves propagate primarily in the $x$ direction.

Even though these simulations have close to a million grid points they run in a few minutes on a serial laptop computer. Rapid simulations with the ability to simulate material interfaces in an accurate, stable and efficient manner opens up the possibility to design multi-physics and multi-scale materials and devices via PDE constrained optimization.

C. Staggered discretization in one dimension for a unit-step modulated sine wave in a linear Lorenz medium

As a final example we perform the experiments from [2] that are depicted in Figures 3 and 4 in that paper. In those experiments a linear Lorenz model with $\omega_0 = 4 \times 10^{16}$ rad/s, $\omega_p = \sqrt{20} \times 10^{16}$ rad/s, $\tau = 0.5/0.28 \times 10^{16}$ is subject to a unit-step modulated sine wave boundary condition at $x = 0$. In Figure 6 we display the same data as in Figures 3 and 4 in [2] for a few different grid resolutions with the 6th order.
note that the results agree qualitatively with those in [2] but that there are slight differences. In particular in the right plot in Figure 6 we note that the right part of the signal is different. Since [2] does not provide much detail of the simulations it is hard to assess how accurate the results in [2] are but as we see grid convergence in our high order accurate simulations we have some confidence that they are correct.

V. Summary

In this paper, we considered the Duffing models for polarization that incorporates both nonlinearity and dispersion. The general $N$th order polynomial Maxwell-Duffing model has an associated energy estimate that guarantees well-posedness of the continuous model, while including polynomial approximations to an exponential Duffing model and also including the linear Lorentz dispersive model as a special case.

We have presented the construction of novel summation by parts finite difference time domain methods (SBP-FDTD) for the numerical discretization of the Maxwell-Duffing models and derived energy estimates for the semi-discrete methods that are analogous to the continuous energy estimates. Even though there is no fully discrete energy estimate, our fully discrete methods based on a variety of time integrators have been shown to preserve a general energy guaranteeing stability of the associated SBP numerical discretizations. In our previous work on energy stable discretizations for Kerr and Raman type nonlinearities [4], [14], we showed that the strength of the nonlinearity in the polarization model does not affect fully discrete energy stability. We intend to perform similar analyses for the Duffing models in future research.

The performance of the proposed SBP-FDTD methods were demonstrated in several numerical experiments. There are many avenues for future research. For example, one can investigate nonlinear optical phenomenon such as third harmonic generation. For example, in one of the numerical experiments we observed that even in the presence of strong nonlinearity, coherent structures, like the standing mode we used as initial data, are robust to the nonlinearity.

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REFERENCES


Daniel Appelö Daniel Appelö holds a M.S. degree in electrical engineering and a Ph. D. degree in Numerical Analysis from the Royal Institute of Technology in Sweden and is currently an Associate Professor in Applied Mathematics at University of Colorado, Boulder.

Vrushali A. Bokil Vrushali Bokil holds a Ph.D. degree in Mathematics from the University of Houston. Bokil is currently a full Professor at Oregon State University in Corvallis, OR, USA.

Yingda Cheng Yingda Cheng holds a Ph.D. degree in Applied Mathematics from Brown University. Cheng is currently an associate Professor at Michigan State University, East Lansing, MI.

Fengyan Li Fengyan Li holds B.S. and M.S. degrees in Computational Mathematics from Peking University and a Ph.D. degree in Applied Mathematics from Brown University. Li is currently a full Professor at Rensselaer Polytechnic Institute, Troy NY USA.